C:\Program Files\Stnexp\Queries\10540519.str

```
102 103 104 105
                  106
                      107 109
                               110
                                   112
ring nodes :
   1 2 3
            5
              6 7 8
                      9
                        10
                            11
                               12 27 28 29 30 31 32 33 34 35 36 37 38 39 40
```

41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61

chain nodes :

71 72 73 74 75 76 77 78 79 80 65 66 67 68 69 70 chain bonds : 2-15 2-19 3-13 3-18 5-22 5-23 6-17 6-21 12-24 13-14 23-112 24-26 32-91 1-16 1-20 44-93 50-94 56-95 62-96 68-97 74-98 80-99 91-104 92-105 93-106 94-107 95-109 38-92

92 93

94 95 96

39-44

40-41

97 98 99

62 63 64

41-42 42-43

96-110 97-100 98-102 99-103 ring bonds : 1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 27-28 27-32 28-29 29-30

35-36 36-37 37-38 39-40

43-44 45-46 45-50 46-47 47-48 48-49 49-50 51-52 51-56 52-53 53-54 54-55 55-56 57-58 57-62 58-59 59-60 60-61 63-64 63-68 64-65 65-66 66-67 67-68 69-70 61-62 69-74 70-71 71-72 72 - 73 73 - 74 75-76 75-80 76-77 77-78 78-79 79-80 exact/norm bonds : 1-2 1-6 1-16 2-3 2-15 3-4 4-5 5-6 5-23 6-17 23-112 24-26 91-104 92-105 93-106

94-107 95-109 96-110 97-100 98-102 99-103 exact bonds :

30-31 31-32 33-34 33-38 34-35

13 14 15 16 17 18 19 20 21 22 23 24 26 91

1-20 2-19 3-13 3-18 5-22 6-21 12-24 13-14 32-91 38-92 44-93 50-94 56-95 62-96 68-97 74-98 80-99

normalized bonds : $7-8 \quad 7-12 \quad 8-9 \quad 9-10 \quad 10-11 \quad 11-12 \quad 27-28 \quad 27-32 \quad 28-29 \quad 29-30 \quad 30-31 \quad 31-32 \quad 33-34 \quad 33-38 \quad 33$

34-35 35-36 36-37 37-38 39-40 39-44 40-41 41-42 42-43 43-44 45-46 45-50 46-47 47-48 48-49 49-50 51-52 51-56 52-53 53-54 54-55 55-56 57-58 57-62 58-59 59-60 67-68 69-70 69-74 60-61 61-62 63-64 63-68 64-65 65-66 66-67 70-71 71-72 73 - 7475-80 76-77 77-78 78-79 79-80 75-76

G1:Cb,Cy,Hy

G2:[*1],[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 17:CLASS 19:CLASS 19:CLASS 20:CLASS 21:CLASS 21:CLA